A new approximation method for time-dependent problems in quantum mechanics

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Abstract

We propose an approximate solution of the time-dependent Schrödinger equation using the method of stationary states combined with a variational matrix method for finding the energies and eigenstates. We illustrate the effectiveness of the method by applying it to the time development of the wave-function in the quantum-mechanical version of the inflationary slow-roll transition.

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There have been various approaches to the calculation of the time development of the Universe in the early stages of inflation, in which the inflaton field φ evolves from the initial unstable vacuum state in which $\langle\varphi\rangle = 0$ to the final stable vacuum in which $\langle\varphi\rangle = \pm a$, say.

At the level of quantum mechanics the earliest approach [1] used the Hartree-Fock method, which, although not very accurate, does give a qualitative picture of the true time development. Several years later Cheetham and Copeland [2] went beyond the Gaussian approximation by using an ansatz which included a second-order Hermite polynomial. This represented an improvement on the Hartree-Fock approximation, but still did not reproduce the first maximum in $\langle x^2\rangle$ of the exact wave-function. A further attempt to solve this difficult non-perturbative problem involved the use of the linear delta expansion [3]. This was successful to the extent that it stayed close to the exact solution for longer than previous methods, but there seemed to be a barrier to its implementation beyond the first maximum. The results of these various approaches to the calculation of $\langle x^2\rangle$ are shown in Fig. 1, where they are compared with the exact result of Lombardo et al. [4], obtained by Fourier transforming to frequency space and then back again.

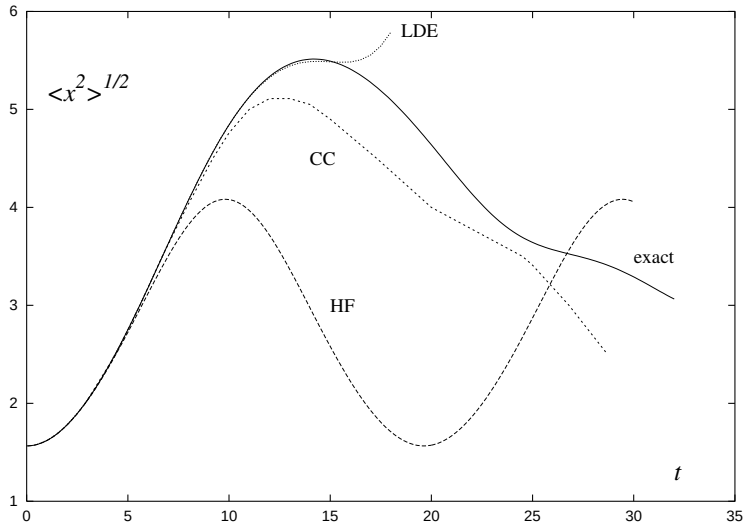

Figure 1: $\langle x^2\rangle^{1/2}$ versus t for the slow roll potential of Eq. (3). The labels HF, CC and LDE correspond to the Hartree-Fock method [1], the improved Hartree-Fock method [2] and the fourth-order linear delta expansion [3] respectively. These are compared with the exact result of [4].

The present paper represents another approach to the problem, using the method of stationary states, combined with a matrix method for finding

the energy eigenvalues of the full Hamiltonian, together with their corresponding eigenfunctions. The method consists of converting the eigenvalue equation into a matrix equation by taking matrix elements with respect to harmonic oscillator wave functions of arbitrary frequency Ω and truncating the matrix at some finite size N. As N increases one may expect the method to become more and more accurate for the lower-lying energy levels. However, for arbitrary Ω the convergence is rather slow. A significant component of our method is to choose an optimal value of Ω by a particular version of the principle of minimal sensitivity (PMS)[5], which greatly accelerates the convergence. The method has been used before for the determination of the eigenvalues[6], but here we also make use of the corresponding wave-functions to implement the method of stationary states to calculate the time-dependence of the state from its initial configuration. It turns out that this simple method is extremely accurate at even quite small orders, and has no difficulty with the long-time behaviour. We have concentrated on this particular problem to exemplify the power of the method, but its range of application is obviously much wider.

As stated above, we tackle the problem of solving the energy eigenvalue equation

$$H\psi_n = E_n\psi_n \tag{1}$$

by converting it to a matrix equation, using an orthonormal basis of wave functions of the quantum harmonic oscillator, depending upon an arbitrary frequency $\Omega \equiv \alpha^2$:

$$\varphi_n(x) = N_n\ e^{-\alpha^2x^2/2}\ H_n(\alpha x)\ , \tag{2}$$

with $N_n = (\alpha/(2^n\ n!\ \sqrt{\pi}))^{\frac{1}{2}}$. The slow-roll Hamiltonian involves a double-well potential, and has the specific form

$$\begin{aligned} H &= \frac{1}{2}p^2 + \lambda(x^2 - a^2)^2/24 + const. \\ &= \frac{1}{2}p^2 - \frac{1}{2}m^2x^2 + gx^4, \end{aligned} \tag{3}$$

with $m^2 = \lambda a^2/6$ and $g = \lambda/24$.

Of course the infinite-dimensional matrix $H_{n\ell}$ must be truncated to some finite dimension, say $N \times N$, and then its eigenvalues can be calculated by simple matrix diagonalization. A brute-force approach to the problem is to stick with a given Ω and rely on larger and larger values of N to approach the desired accuracy for the lower-lying energy levels. However, much improved

accuracy for even modest sized matrices can be obtained by a judicious choice of Ω. The criterion we shall adopt here, which is essentially that adopted in [6], is the principle of minimal sensitivity[5] applied to the trace of the truncated matrix.

The rationale behind this principle is that the eigenvalues and other exact quantities of the problem are independent of Ω but any approximate result coming from the diagonalization method for finite N exhibits a spurious dependence on the oscillator frequency. This also applies to the trace of the matrix, i.e. the sum of the eigenvalues. A well-motivated criterion for choosing Ω is therefore to take it at a stationary point of $T_N \equiv \sum_{n=0}^{N-1} H_{nn}$, so that this independence is respected locally. Thus we impose the PMS condition

$$\frac{\partial}{\partial \Omega} T_N = 0 \ . \tag{4}$$

The reason for applying this condition to the trace is that T_N is a simple quantity to evaluate, and moreover it is invariant under the unitary transformation associated with a change of basis. Once Ω is so determined, one obtains an approximation to the first N eigenvalues and eigenvectors of H by a numerical diagonalization of the truncated $N \times N$ matrix. One could also contemplate applying the PMS to the determinant, which of course shares the property of invariance under unitary transformations, but this would be a much more cumbersome calculation, and could well introduce many spurious PMS solutions.

In order to implement the method we need the harmonic oscillator matrix elements of x^p. Closed formulas have been given in Ref. [7], which we adapt here for completeness.

$$(x^{2r})_{n\ell} = \frac{\sqrt{n!\ell!}}{(2\alpha)^{2r}} \sum_{k=0}^{\min(n,r-\lambda)} \frac{(2r)!}{2^{2r-k-\lambda}(r-\lambda-k)!(n-k)!(2\lambda+k)!k!} \tag{5}$$

for $\ell - n = 2\lambda$, and

$$(x^{2r+1})_{n\ell} = \frac{\sqrt{n!\ell!}}{(2\alpha)^{2r+1}} \sum_{k=0}^{\min(n,r-\lambda)} \frac{(2r+1)!}{2^{2r-k-\lambda+\frac{1}{2}}(r-\lambda-k)!(n-k)!(2\lambda+1+k)!k!} \tag{6}$$

for $\ell - n = 2\lambda + 1$. These formulas assume $\ell \geq n$, but the matrix is symmetric. In both cases r must be greater than λ. For all other values of p, n and ℓ the matrix elements vanish.

In addition to these we will need the matrix elements of p^2, which are given by

$$(p^2)_{n\ell} = -\frac{1}{2}\alpha^2 \left[\sqrt{\ell(\ell-1)}\delta_{\ell,n+2} - (2\ell+1)\delta_{\ell,n} + \sqrt{(\ell+1)(\ell+2)}\delta_{\ell,n-2}\right]. \quad (7)$$

Using these results we can write down the matrix elements of Eq. (3) in the basis of the wave functions of Eq. (2). The trace to order N is given by

$$\frac{4}{N}T_N = N(\Omega + \frac{m^2}{\Omega}) + \frac{g}{\Omega^2}(1+2N^2), \quad (8)$$

which turns out to have a single minimum, located at

$$\Omega_{PMS} = \frac{1}{3}X^{1/3} - \frac{m^2}{X^{1/3}}, \quad (9)$$

where

$$X \equiv \frac{3}{N}\left[9g(1+2N^2) + \sqrt{3}\left(N^2m^6 + 27g^2(1+2N^2)^2\right)^{\frac{1}{2}}\right] \quad (10)$$

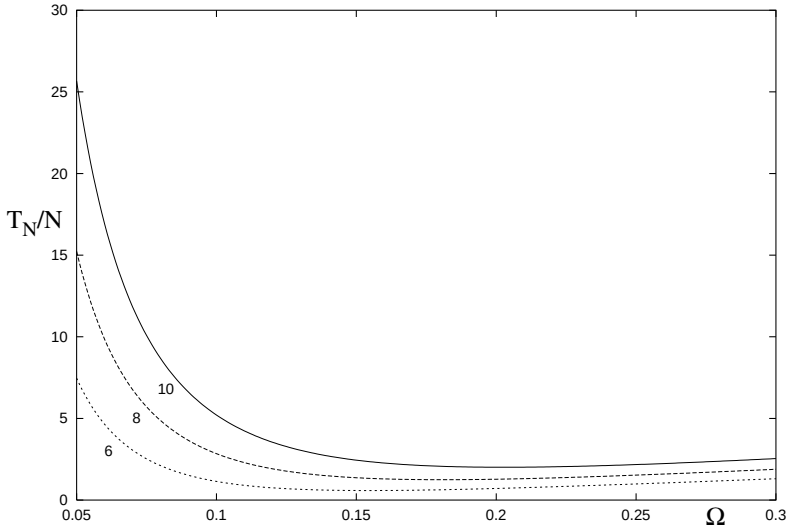

Figure 2: Trace of the truncated matrix for the Hamiltonian (3) normalized by the number of states as a function of the variational parameter Ω for $a = 5$, $\lambda = 0.01$. The three curves are for $N = 6$, 8, 10.

A graph of T_N/N against Ω is given in Fig. 2 for various values of N. Here we have taken the parameters as $a = 5$, $\lambda = 0.01$, in accordance with previous

work on the subject[1, 2, 3]. By taking Ω at the minimum, in accordance with PMS, we obtain a good approximation to the spectrum for even quite small matrices.

For the present purposes, the important point of this method is that in addition to the energy levels it gives an approximation to the energy eigenfunctions, in the form

$$\psi_n(x) = \sum_{k=0}^{N-1} d_{nk}\ \varphi_k(x)\ . \tag{11}$$

where d_{nk} denotes the kth component of the nth eigenvector of the truncated Hamiltonian matrix.

These can be used to implement the method of stationary states. Namely, if the initial wave-function at $t = 0$ is expanded as

$$\Psi(x,0) = \sum_{n=0}^{\infty} a_n \psi_n(x), \tag{12}$$

its value at a later time is given by

$$\Psi(x,t) = \sum_{n=0}^{\infty} a_n\ e^{-iE_n t}\ \psi_n(x) \tag{13}$$

As an intermediate step we expand $\Psi(x,0)$ in terms of the eigenvectors $\varphi_n(x)$:

$$\Psi_n(x,0) = \sum_{k=0}^{N-1} c_n\ \varphi_n(x)\ . \tag{14}$$

By comparison with Eq. (12) we see that

$$a_n = \sum_{\ell=0}^{N-1} c_\ell\ (\mathbf{d}^{-1})_{\ell n}\ . \tag{15}$$

Notice that by this stage Ω has been determined by the PMS condition, so that the matrix inversion here is numerical, rather than symbolic.

It remains to determine the coefficients c_n in Eq. (14). The initial wave function used in previous studies of slow-roll inflation is given by

$$\Psi(x,0) = \left(\frac{m}{\pi}\right)^{1/4} e^{-mx^2/2}.$$

By orthonormality,

$$c_n = \int \phi_n^*(x)\Psi(x,0)dx = N_n\ \left(\frac{m}{\pi}\right)^{1/4}\ \int_{-\infty}^{+\infty} e^{-\beta^2 x^2/2} H_n(\alpha x)dx, \tag{16}$$

where $\beta^2 \equiv m + \alpha^2$. By means of the change of variable $y = \alpha x$

$$c_n = \frac{N_n}{\alpha}\left(\frac{m}{\pi}\right)^{1/4} \int_{-\infty}^{+\infty} e^{-\frac{\beta^2}{2\alpha^2}y^2} H_n(y) dy \ . \tag{17}$$

and the expansion of $H_n(y)$, namely

$$H_n(y) \ = \ \sum_{k=0}^{[n/2]} (-1)^k \frac{n!}{(n-2k)!k!} 2^{n-2k} y^{n-2k} \ . \tag{18}$$

we obtain

$$c_n \ = \ \frac{N_n}{\alpha}\left(\frac{m}{2\pi}\right)^{1/4} \sum_{k=0}^{[n/2]} (-1)^k \frac{n!}{(n-2k)!k!} 2^{n-2k} \ J_k, \tag{19}$$

where

$$J_k \ \equiv \ \int_{-\infty}^{+\infty} y^{n-2k} e^{-\frac{\beta^2}{2\alpha^2}y^2} dy = \left(\frac{\sqrt{2}\alpha}{\beta}\right)^{n-2k+1} \ \int_{-\infty}^{+\infty} z^{n-2k} \ e^{-z^2} dz \ .$$

In fact $c_n = 0$ unless n is even $n = 2\ell$, and then

$$c_{2\ell} \ = \ \frac{N_{2\ell}}{\alpha}\left(\frac{m}{\pi}\right)^{1/4} \sum_{k=0}^{\ell} (-1)^k \frac{(2\ell)!}{(2\ell-2k)!k!} 2^{2(\ell-k)} \left(\frac{\sqrt{2}\alpha}{\beta}\right)^{2(\ell-k)+1} \Gamma\left(\ell - k + \frac{1}{2}\right). \tag{20}$$

The coefficients a_n are now given by Eq. (15).

For comparison with previous work, we use our time-dependent wave function to calculate $\langle x^2 \rangle$, given by

$$\langle x^2 \rangle \ = \ \int \Psi^*(x,t) \ x^2 \ \Psi(x,t) \ dx \tag{21}$$

assuming that $\Psi(x,t)$ remains normalized, which we have checked. In terms of the $\psi_n(x)$ this is

$$\langle x^2 \rangle \ = \ \sum_{n,\ell} \ a_n^* \ a_\ell \ e^{-i\omega_{n\ell}t} \ \int \psi_n(x) \ x^2 \ \psi_\ell(x) \ dx, \tag{22}$$

where $\omega_{n\ell} \equiv E_n - E_\ell$. Using Eq. (11) this becomes

$$\langle x^2 \rangle = \sum_{n,\ell} \ a_n^* \ a_\ell \sum_{k,j} d_{nk} d_{\ell j} (x^2)_{kj} \ \cos\omega_{n\ell} t \ . \tag{23}$$

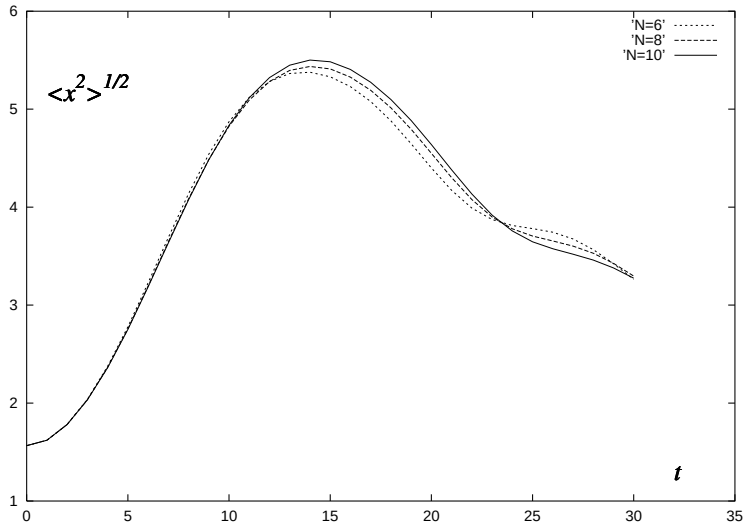

Figure 3: $\langle x^2 \rangle^{1/2}$ versus t for the slow roll potential of Eq. (3) calculated with our method for N=6, 8 and 10. On the scale of the figure, the result for N=10 is barely distinguishable from the exact result.

The result for $\langle x^2 \rangle^{1/2}$ is plotted in Fig. 3. As can be seen, the method is vastly superior to the previous approximative methods, and by $N = 10$ the curve can hardly be distinguished from that obtained using Fourier transform methods. Although for the present purposes a basis of size 10 was sufficient, considerably greater accuracy for both energies and eigenfunctions can readily be obtained by going to larger N. This costs little additional effort because, once the PMS has been applied, the Hamiltonian matrix is fully numerical and the calculation of its eigenvalues/eigenvectors can be calculated numerically with accuracy and speed. For example, with $N = 100$ we obtain the energy of the ground state of the quartic oscillator Hamiltonian $p^2 + x^2 + 2gx^4$ with $g = 1000$ to an accuracy of 58 significant figures. Although we have no analytic proof, our numerical work strongly suggests that the error decreases exponentially with N.

In both these cases we have been dealing with symmetric potentials, but with a slight modification it can easily be extended to asymmetric potentials. In such a case, instead of using a basis of harmonic oscillator wave-functions centered on the origin, we can take them to be centered on a shifted position $x = \sigma$. The method then contains two variational parameters Ω and σ, which are to be determined by the PMS condition that T_N be stationary in both.

Another possible extension of the method might be to use the eigenfunc-

tions of the q-deformed harmonic oscillator as a basis instead of those of the simple harmonic oscillator. A variational method using these eigenfunctions has been shown to give very accurate results for the ground-state energy of the anharmonic oscillator[8].

In conclusion, we have shown that the matrix method, combined with the principle of minimal sensitivity applied to the trace of the Hamiltonian matrix, is a powerful tool for finding the spectrum of arbitrary polynomial potentials having only bound states. Since the method also gives the energy eigenfunctions it is ideal for implementing the method of stationary states in order to track the time development of a given initial wave function. For quite modest-sized matrices the method gives good accuracy, even for long time scales, as we have demonstrated for the slow-roll potential.

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